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A Sampling of Multiscale Material Simulation at Sandia National Laboratories

"Microsystems and Beyond"

Sandia Science Day

24 June 2002

John B. Aidun, Manager
Computational Materials and Molecular Biology, 9235

CCIM
COMPUTATION, COMPUTERS, INFORMATION AND MATHEMATICS
National Leadership in High Performance Computing

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories

Sandia: The Extreme Engineering Lab

Extreme sports athlete
Dave Mirra

To fulfill our National Security mission, we develop systems and components designed to perform extreme applications, under adverse conditions.

The duty cycle can include damage, crush and failure;

melting; decomposition – or just plain old age.

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Example Applications I

Extremely Tough:

- Earth penetrator bombs
- Radiation-hard microelectronics
- Explosive Destruction System

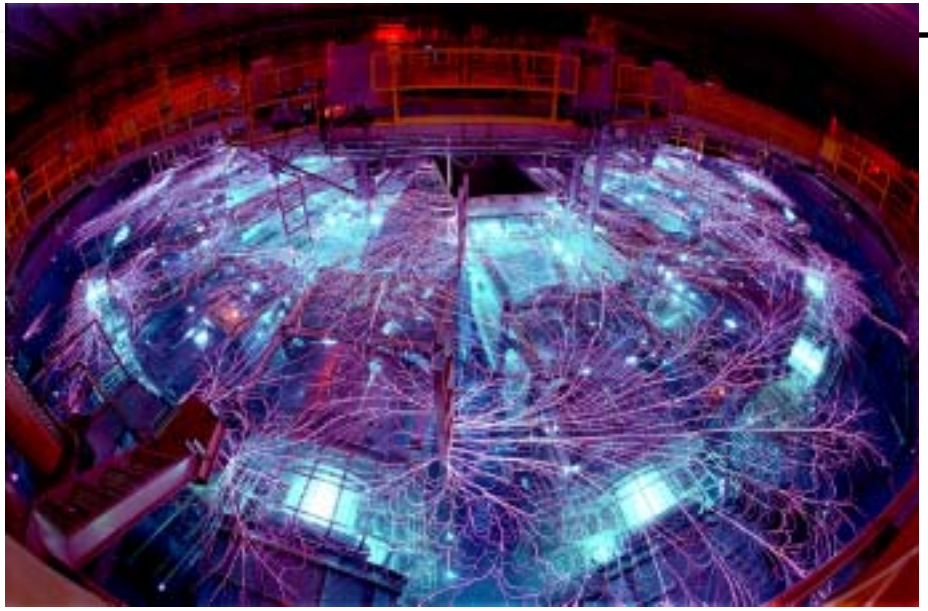
Extremely Sensitive:

- Sensors
- Explosives Sniffer

Extremely Powerful:

- Ferroelectric ceramic power supply
- Pulsed Power Z-Machine

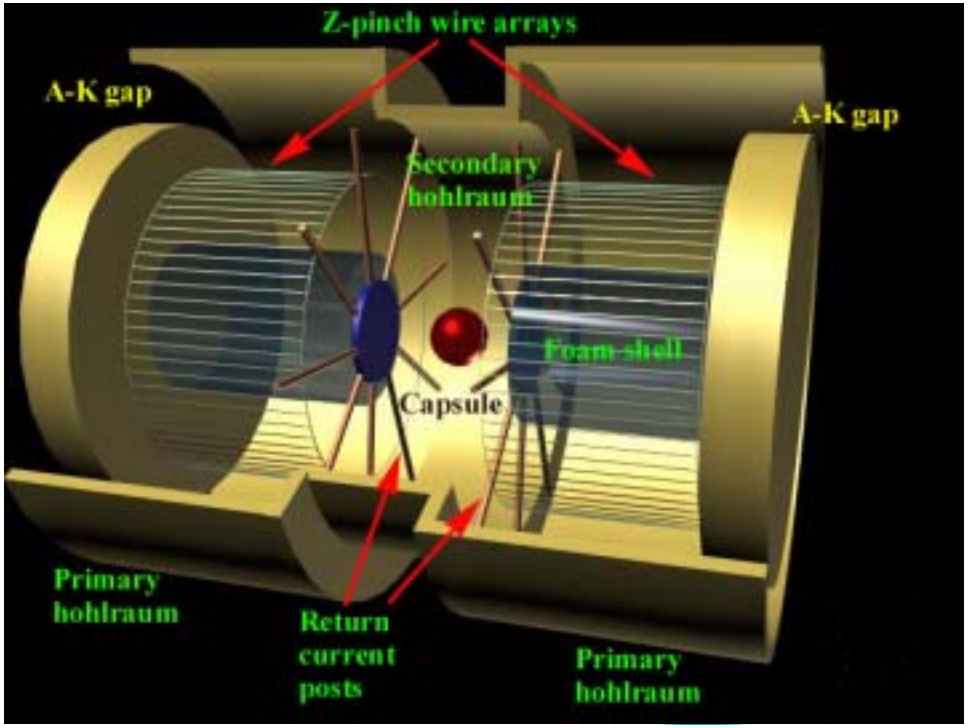
Pulsed Power & Inertial Confinement Fusion (ICF)



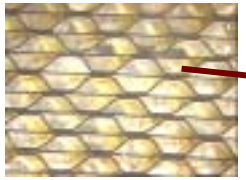
- ICF is a goal at Sandia National Labs
- Pulsed Power Technique using Z-machine

Wire arrays explode, creating a plasma sheath, which implodes and stagnates.

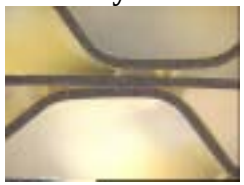
Resulting X-rays strike capsule, generating fusion reaction.

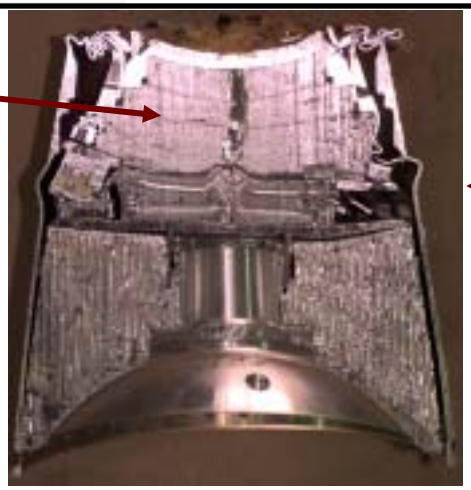


Example Applications II



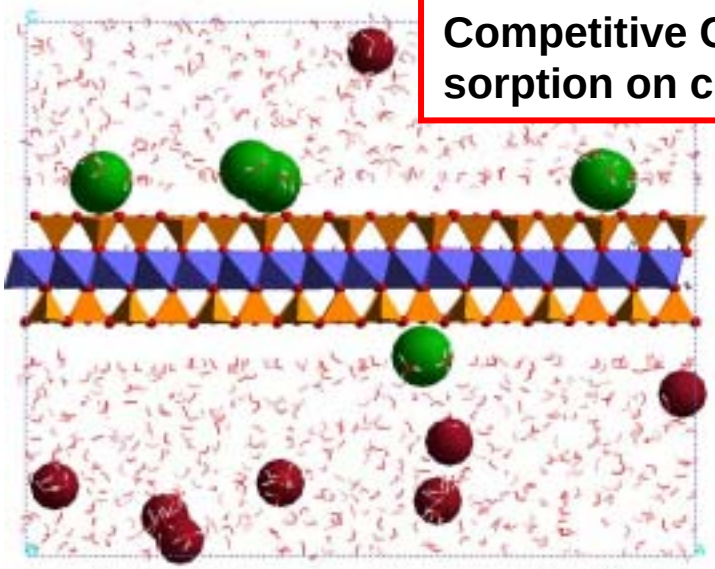
Aluminum Honeycomb





Extreme Insult Resistant:

- Aluminum Honeycomb energy absorber
- Engineered Stress Profile Glass
- Architectural Surety



Competitive Cs and Sr sorption on clay mineral

Extreme Effectiveness:

- Environmental remediation
- Decontamination Foam

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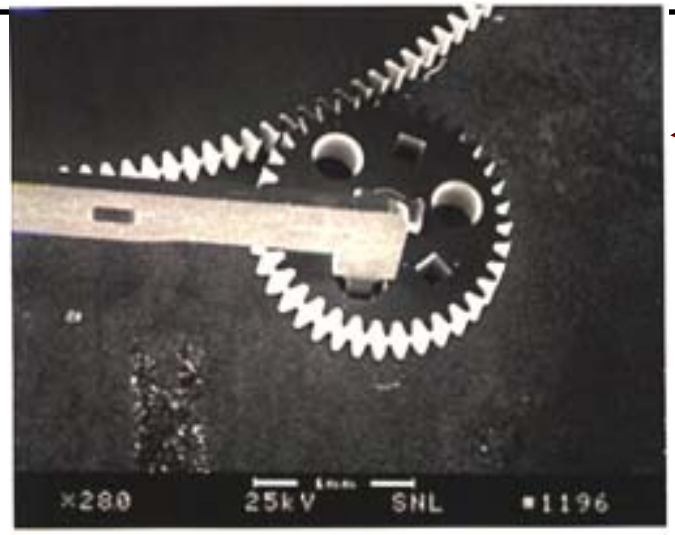
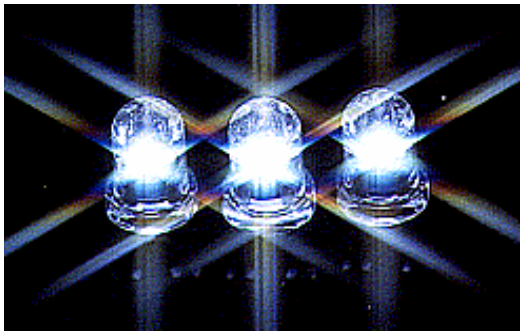
Example Applications III



Extremely Small & Efficient:

- Microsystems & Nanotechnology
- Solid State Lighting



Extremely Reliable:

- Electrical Connectors
- Bonds
  - Solder Joints
  - Adhesives Joints
  - Brazes and Welds

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Sandia: A Materials & Engineering Lab

- Extreme Engineering requires understanding and controlling the properties and behavior of materials.
  - In turn, this often requires understanding and controlling processing, which determines many aspects of material performance.
- Consequently, materials research is a big part of Sandia's Science & Technology efforts.
- **Computer modeling and simulation** is an integral part of the materials research we pursue.
  - It goes hand-in-hand with theory, experimentation, synthesis, and measurement.

Drivers for Ever-Increasing Goals for Materials Performance

- Continually evolving National Security needs .
- Technological Goals:
  - Smaller; Lighter
  - Higher Speed; Higher Efficiency; Higher Sensitivity
  - Greater Economy
  - More versatile; More robust in severe environments
- To meet new performance goals, we increasingly look to computer modeling & simulation to quickly provide accurate information on properties and behavior of materials, *both existing and imagined*.

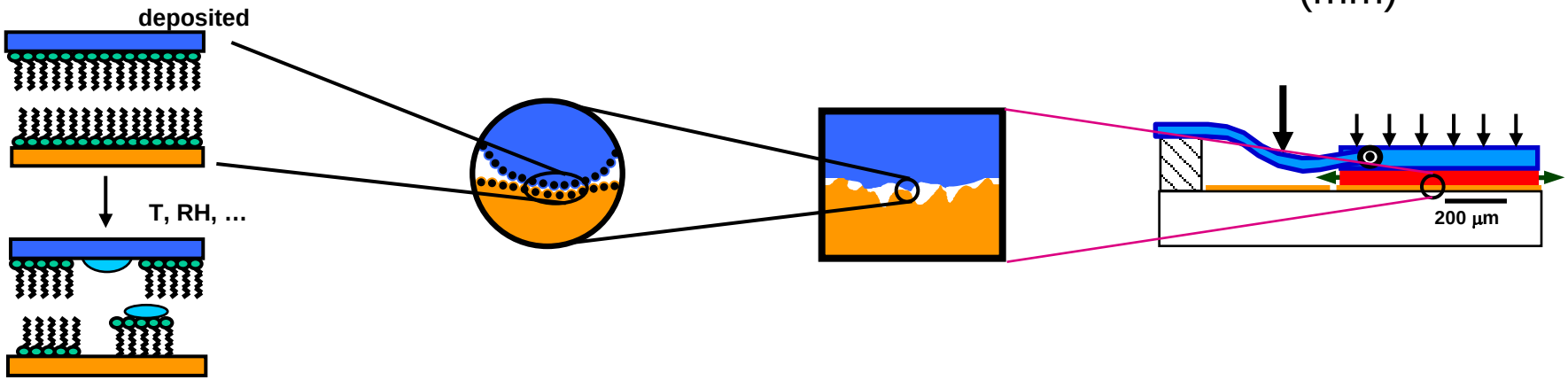
Why Multiscale Material Simulation?

- The **GOAL** for materials modeling & simulation is to be able to make good predictions for **REAL** materials.
- Need to identify & understand the fundamental events occurring in each material (type) for each application.
- Primary physical traits and chemistry are determined at the atomistic level.
- Each scale of **heterogeneity** introduces additional phenomena
  - Lattice Defects; Subgrain domains; Grain boundaries; Multiple phases; Micro-cracks

Multiscale Material Phenomena – Interfacial Forces in MEMS

Linking length scales needed to understand and model adhesion, friction and wear:

Å → nm → μm → Micromachines (mm)



- SAM coatings
- molecular structure
- stability and durability
- environmental degradation

- single asperity
- adhesion energy
- friction coefficient
- dynamics
- atomistic simulation

- multi-asperity
- surface morphology
- 'real' contact simulation

- design rules
- device models
- device performance
- reliability testing

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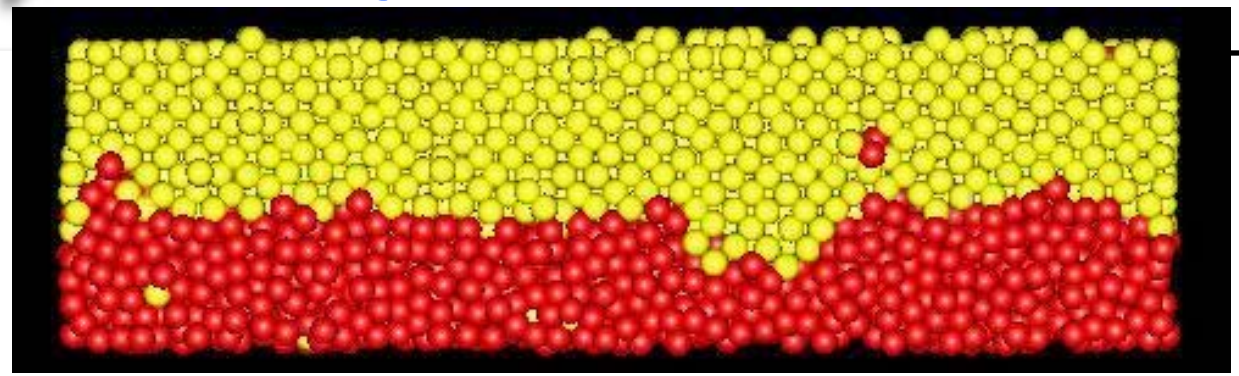
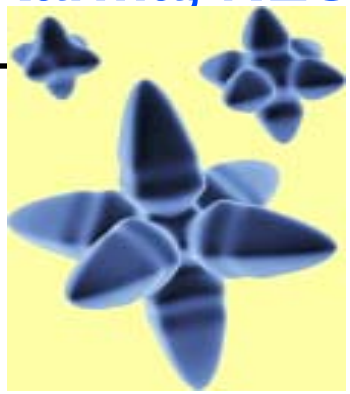
Sequential multiscale prediction of solidification rates in Ni

Jeff Hoyt, SNL; Mark Asta, NWU; Alain Karma, NEU

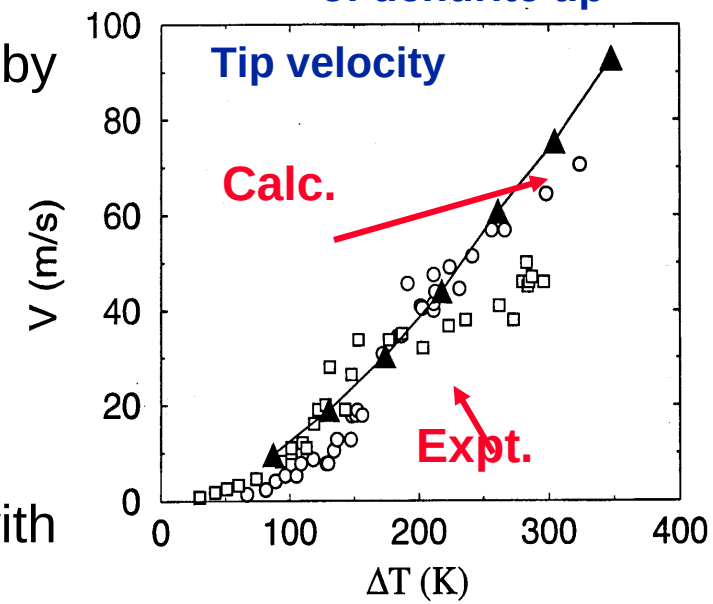


MD simulation of liquid-solid interface



Phase-field simulation of dendrite tip

- Molecular Dynamics simulations of solid-liquid interface predict parameters needed by phase-field model
  - Anisotropic interfacial free energy
    - *Novel fluctuation analysis*
  - Kinetic coefficients
- EAM potentials of Foiles, Baskes and Daw
- *Parameter-free* phase-field calculations predict dendrite tip velocity in agreement with experiment



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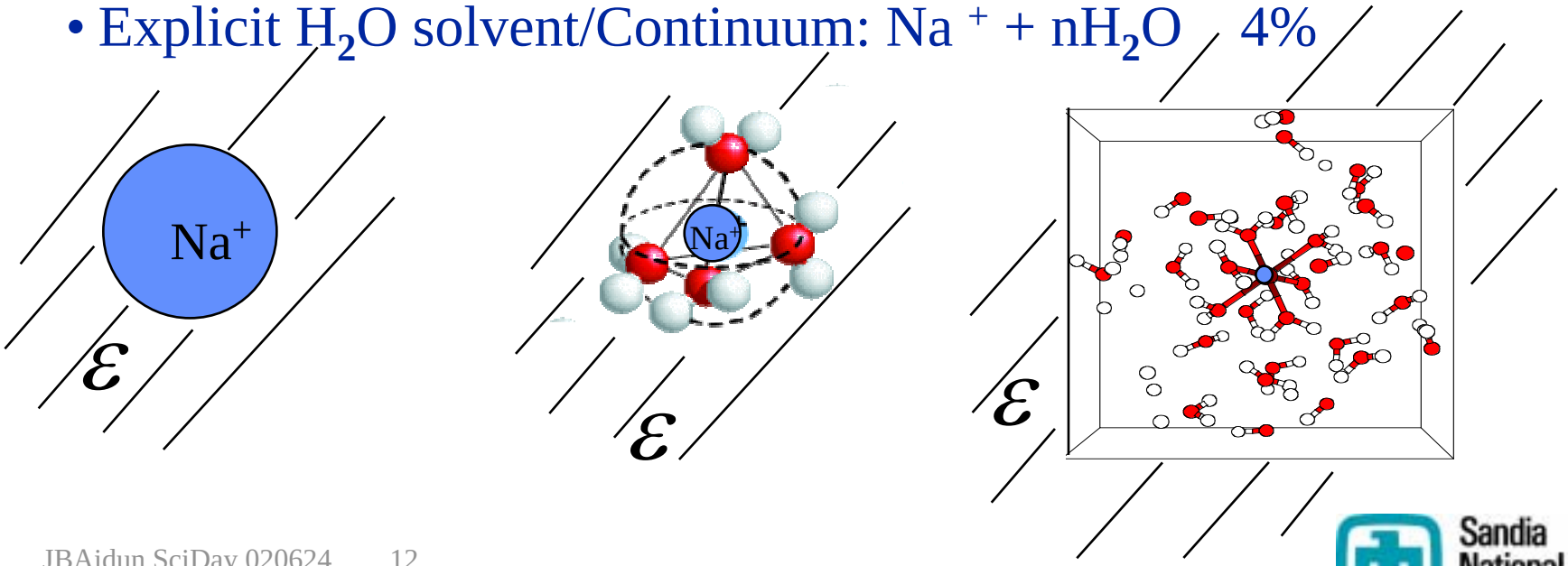
Concurrent multiscale prediction of Hydration Energy for Sodium

S. Rempe (SNL), D. Asthagiri, L. Pratt (LANL), 2002

	$\Delta E^{hydration}$ Error
• Dielectric Continuum: $Na^+(aq)$	40%
• Explicit bound H_2O molecules: $Na^+ + nH_2O$	30%
• Explicit bound H_2O/Continuum: $Na^+ nH_2O$	15%
• Explicit H_2O solvent/Continuum: $Na^+ + nH_2O$	4%



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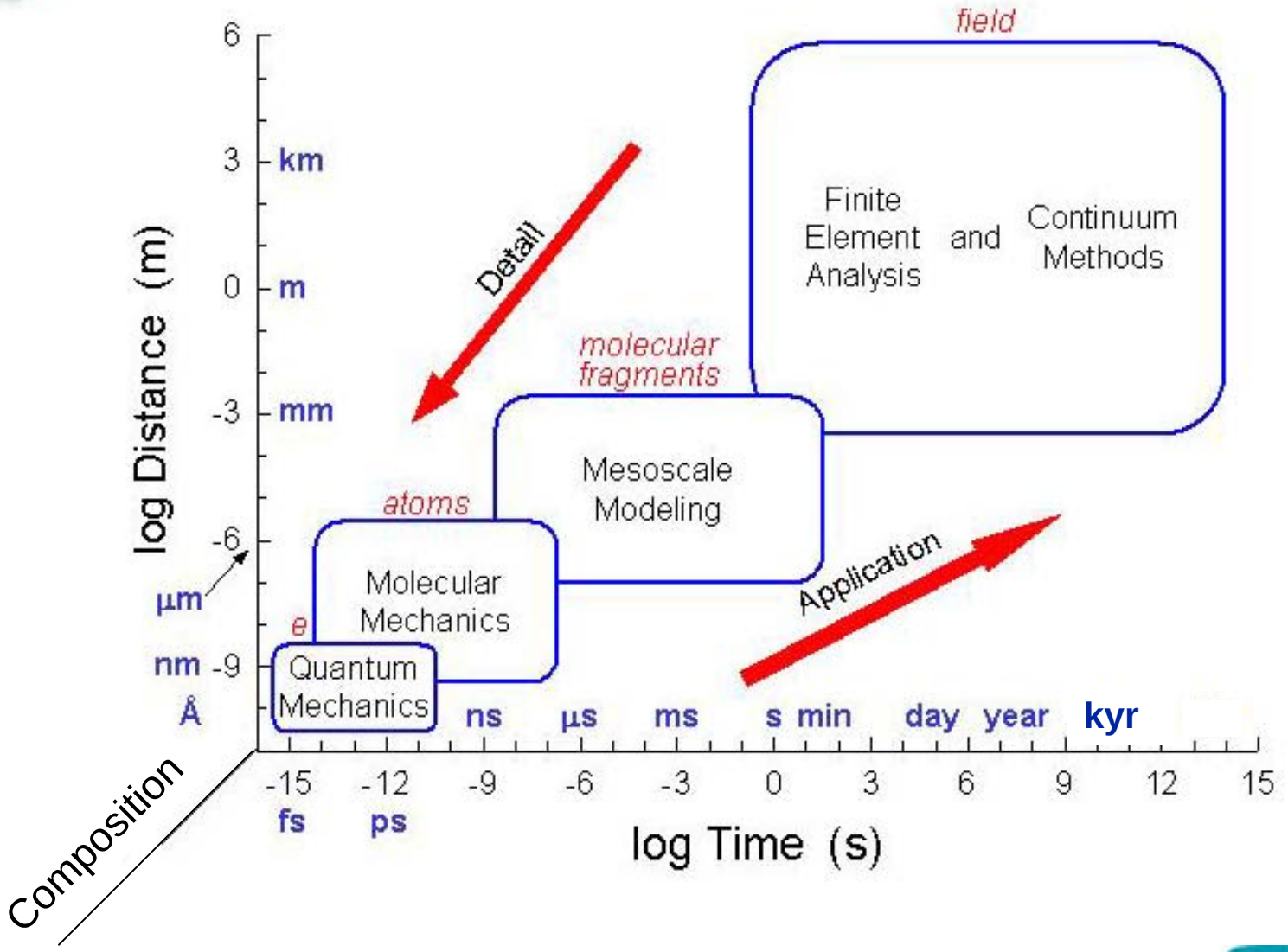
The Challenge: Size, Time, & Number

- Atoms to Objects:
  - nanometers, femtosec → cm, sec, Giga-Giga atoms
  - years: 10's of Msec
- Brute Force – State of the Art: F.F. Abraham (IBM)
  - 1 Billion atoms (Giga atom); a speck less than 1 μm^3
  - Highly simplified atomic interaction
  - Time interval 0.1 ns to 10 ns
- Moore's law will gradually extend the range of brute force.
- But brute force will never address the more subtle challenges associated with heterogeneity (next)

The Deeper Challenge to Multiscale Materials Simulation – The need for Science

- Capturing diffusion, reactivity, and chemistry
  - This often requires Quantum Mechanics accuracy
- Attaining effectively very long times – Aging studies
- Applying high accuracy techniques when and where they are needed within a large system
  - "Interesting" events are infrequent.
  - Their time and location are not known.
- Removing or suppressing disturbances made by artificial boundaries in atomistic simulations.
  - Nanoscience is an easier target, in some ways.
  - Periodic Boundary Conditions – easy, but limited

Computer Simulation L-t-x Array



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Classes of Simulation Methods

Quantum (nm, ps)

- Q.Monte Carlo
- Q.Density Functional Theory
- Tight Binding

Molec. Modeling (mm,ms)

- Molecular Dynamics
- Atomistic Monte Carlo (MC)
- Molecular Statistical Theory

Mesoscopic (mm, s)

- Dislocation Dynamics
- Lattice Gas
- Cellular Automata
- Kinetic MC/Potts
- Coarse Grained MD
- Phase Field Models

Continuum down to (μm, μs)

- Finite Element Method
- Finite Difference
- Boundary Element
- Finite Volume
- Particle-in-Cell
- Transform methods

Green: PDE methods

Meeting the Challenge of Multiscale: Coupled Methods

- Solutions to the technical challenges are being sought in coupling simulation methods
  - Concurrent coupling / strong coupling needed for tightly coupled problems
    - *Fracture; Electrical Breakdown; Superconductivity; HE Detonation; protein folding & activity; other Biology*
  - Sequential / hierarchical coupling often suffices
    - *Characteristic Lengths & Times do not overlap*

- The essential scientific challenge in coupling simulations is making the transition to the coarser scale
  - Must capture the dominant physical processes -- and not more.

Coupled Simulation Methods as BCs

- Couple methods together tightly to use the coaser, less accurate method as boundary constraints (BC) for the higher accuracy method
  - FEM mesh of a continuum as BC for MD
  - Classical MD as BC for Quantum
  - Molecular Continuum as BC for Quantum

Coupled Simulation Methods: Transitions

- Scientific insight is required to devise the needed Transitions between scales and methods:
  - Discrete to thermomechanical Continuum
  - Quantum to Classical
  - Deterministic to Statistical/Stochastic

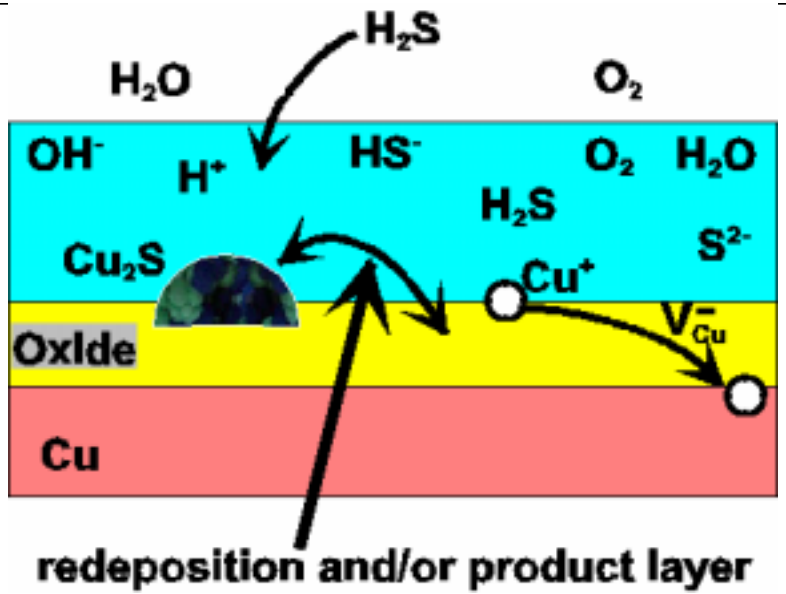
Developing Coupled Methods to capture Chemistry & Thermomechanics

- Highlight 4 current Sandia projects
  - Modeling Atmospheric Corrosion of Electrical Devices (PI Stephen Foiles, 1834)
  - Developing Multiscale and Reactive Force Field Methods (PI Peter Schultz, 9235)
  - Modeling Local Chemistry in the Presence of Collective Phenomena (PI Normand Modine, 1112)
  - A Coupled Approach for Atomistic-Continuum Simulation (PI Jonathan Zimmerman, 8726)

Simulating Chemistry

- Current Challenge: Extending force fields to describe reactions (bond breaking and formation)
  - Stephen's approach:
    - *Sequential knowledge transfer. Understanding from atomistic study used to guide modeling in the continuum.*
    - *traditional approach to take for multi-process and rich phenomena.*
  - Peter's approach:
    - *Devise force fields that are reactive*
    - *Fix the parameters using QM calculated "data"*
  - Normand's approach:
    - *Tightly couple QM & MD*
    - *Describe the reaction center quantum mechanically*
    - *Rely on the MD region to capture collective phenom.*

Modeling Atmospheric Corrosion of Electrical Devices – S. Foiles



Use Atomistic Simulations and Experiments to generate needed Subgrid-Physics Models

3D multi-phase reaction/diffusion continuum model is needed to simulate real devices and geometry

Multiple Phenomena:

- Adsorption,Speciation, and Reactions, Transport in Liquid Layer
- Gas Phase Transport and Environment
- Liquid Solid Surface Reactions
- Multi-layer solid-state Diffusion

Length Scales:

- Devices (1000 μm)
- Sulfide (1 μm)
- Oxide (0.01 μm)
- Water (0.001 μm)

Time Scales:

- Devices (10^9 sec)
- Atomic (10^-12 sec)

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Microscopic understanding used to define the continuum level models

- Surface reaction rates – control of stage I kinetics
  - Form of the constitutive law for surface reactions determined by the microscopic mechanism
  - Need to understand chemistry in *nanoscale* aqueous layers
- Solid State transport – control of stage II kinetics
  - Point defect properties and standard kinetic models
    - *Complex crystal structures makes this very challenging*
    - *Role of impurities?*
- Some unanswered questions for microscopic models
  - Mechanistic origins of corrosion product morphology
  - Explain experimentally observed variation of rates with
    - *Relative humidity*
    - *Light levels*

Significant Challenges at the Continuum Level

- Electrical device-scale simulations performed with ARIA, a 3-D, multiphase, continuum reactive transport code
- Computational challenges for continuum code
  - Multiple phases; Corrosion product morphology
  - Moving boundaries; Globally-dependent reactions
  - Widely disparate length scales and *Long Times*
- Treatment of uncertainty and variability
  - Model/parameter uncertainty and variation in the environment
  - Continuum equations are deterministic for a specific environmental history, initial state, and parameters
    - *Deterministic simulation for a realistic 3D geometry is time-consuming.*
    - *Need to determine probability of failure as a function of time.*

Developing Multiscale and Reactive Force Field Methods - P. Schultz

Aim: Integrate atomistic simulation methods to invest fast, versatile semi-empirical methods (MD, TBMD) with quantum accuracy.

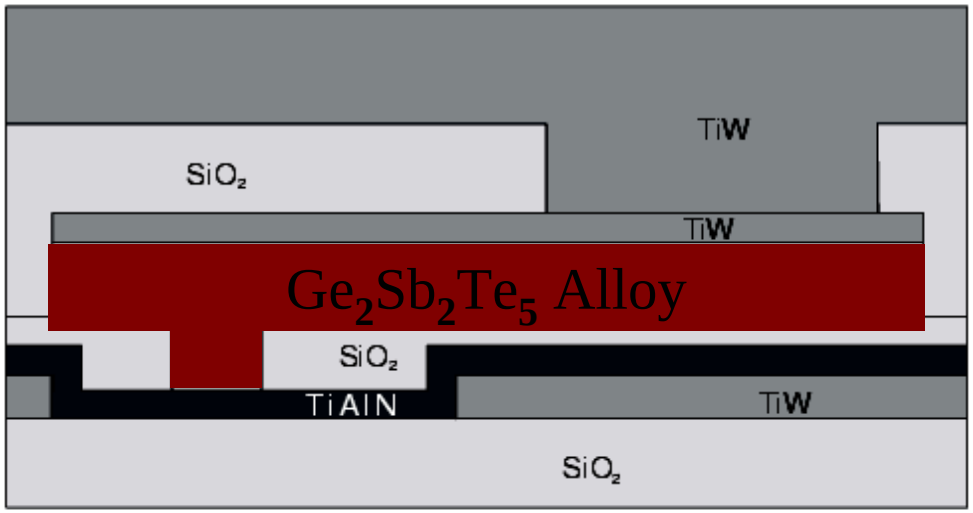
Result: A multiscale materials simulation problem-solving framework and know-how to make use of it.

Test Case: Phase Change Memory Technology

- Non-volatile, Radiation-Hard Memory needed for DOE and Air Force microelectronics applications.
- Electrical analog of optical memory used in CD RW, DVD-RAM and DVD+RW media.
- Small spots of $Ge_2Sb_2Te_5$ alloy rapidly switched between amorphous and crystalline phases.

Non-Volatile C-RAM

- **Simple planar offset structures have been used to investigate basic device physics**



- High endurance
- Long data rentention
- Low voltage, low power
- Compatible with Si chip technology
- Highly scalable
- Enables logic + memory system-on-a-chip

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Target Physics & Chemistry Issues for C-RAM Simulations

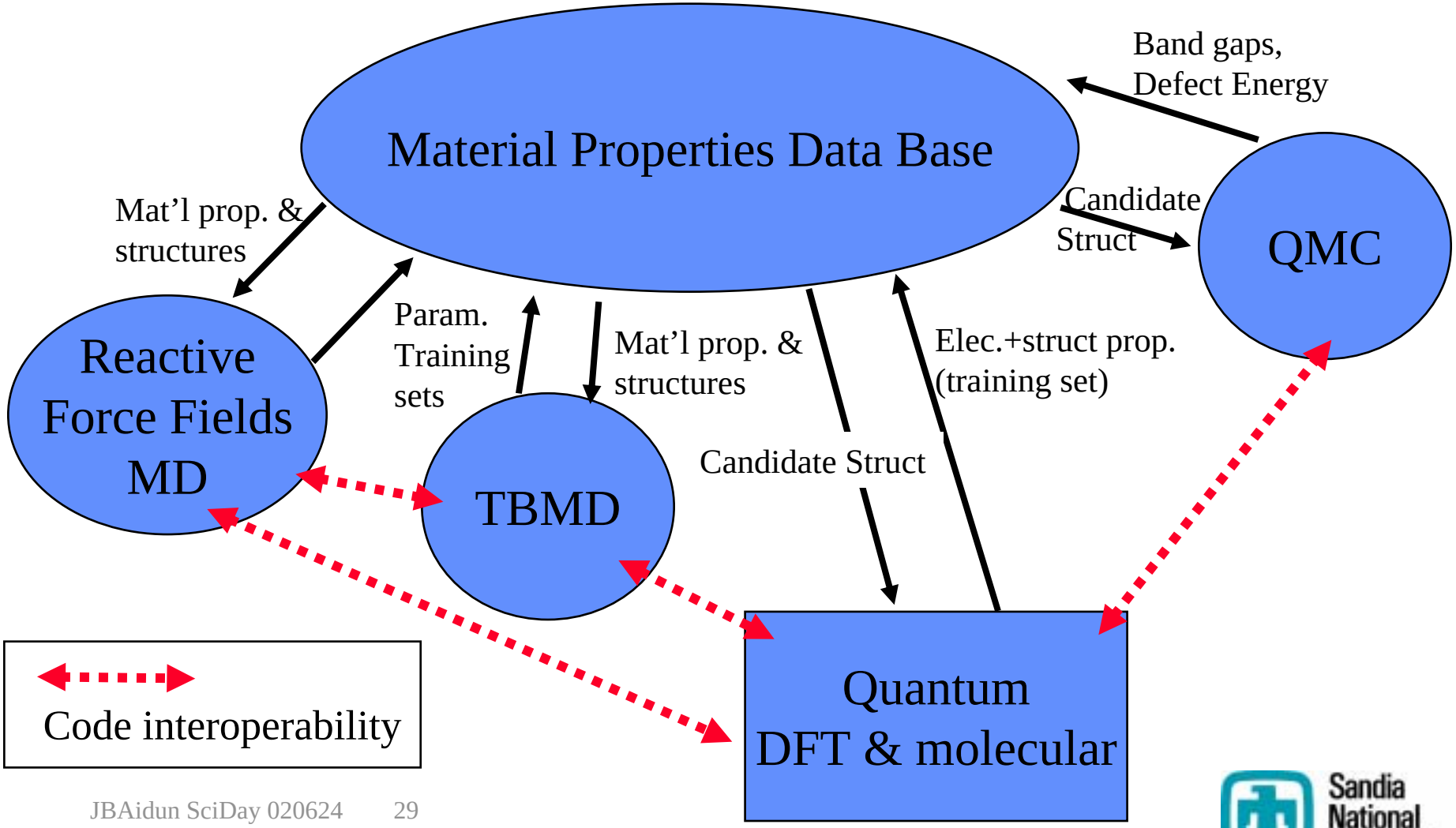
- The Phase Transitions
  - Structural: amorphous to poly-crystalline
  - Electronic: semiconducting to metallic
- Switching time (10's of nanoseconds)
- Macroscopic response
  - Delamination?
  - Material compatibilities?

The Material Modeling Process

Development and parameterization of RFF MD & TBMD:

1) Choose the physics needed in the simulation.
2) Identify atoms and other particles.
3) Choose parameterization of the physics.
4) Generate Training Sets of material property values ("data")
5) Perform internal validation.
6) Apply calibrated semi-empirical method.
7) Augment with full quantum calculations, where needed.

Material Modeling Tool Set



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Challenges to Simulating C-RAM

- Complex physics
  - Phase transitions: Structural & Electronic
    - *Likely to be coupled → electronic/thermally driven*
  - Electronic properties are critical for accuracy
  - Extended time scale (10's of ns): pushes ability of classical MD; beyond the range of TBMD
- Simulation Methods
  - New formulations for force fields to portray the Chemistry
  - New multi-component/multi-phase TBMD
  - Codes need to be interoperable (loosely coupled)
  - Big simulations needed in QM, TBMD, and MD

Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

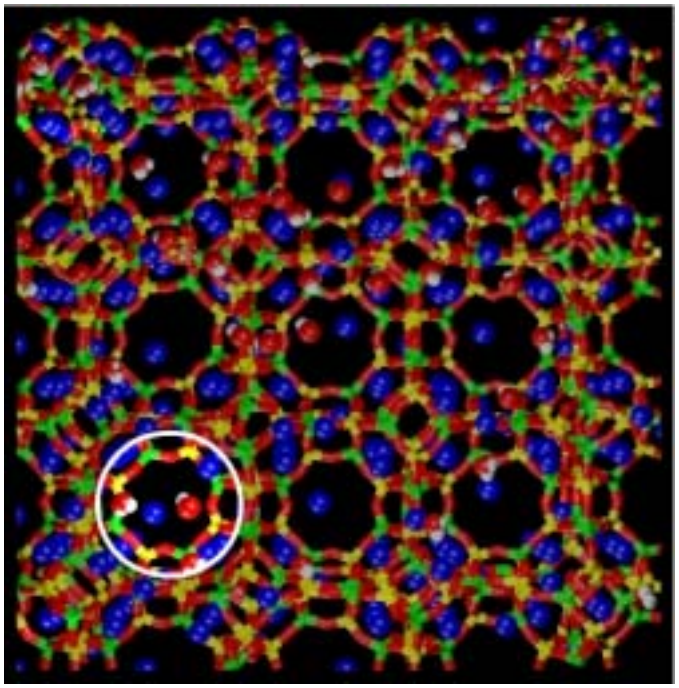
Aim: Model local Chemistry in the presence of Collective Phenomena to advance scientific understanding of complex materials

Test case: Absorbtion in Zeolite desiccant

Approach: Couple Green's Function Electronic Structure method to classical MD

- Exploits localized nature of ES.
- Transition: "anchored" orbital BC on QM region facilitate embedding in classical MD region.
- Update ion positions in QM region after every MD time step.

Result: A flexible, production-level multiscale modeling tool for materials science.



Zeolite: nano-porous alumino-silicate + Na^+

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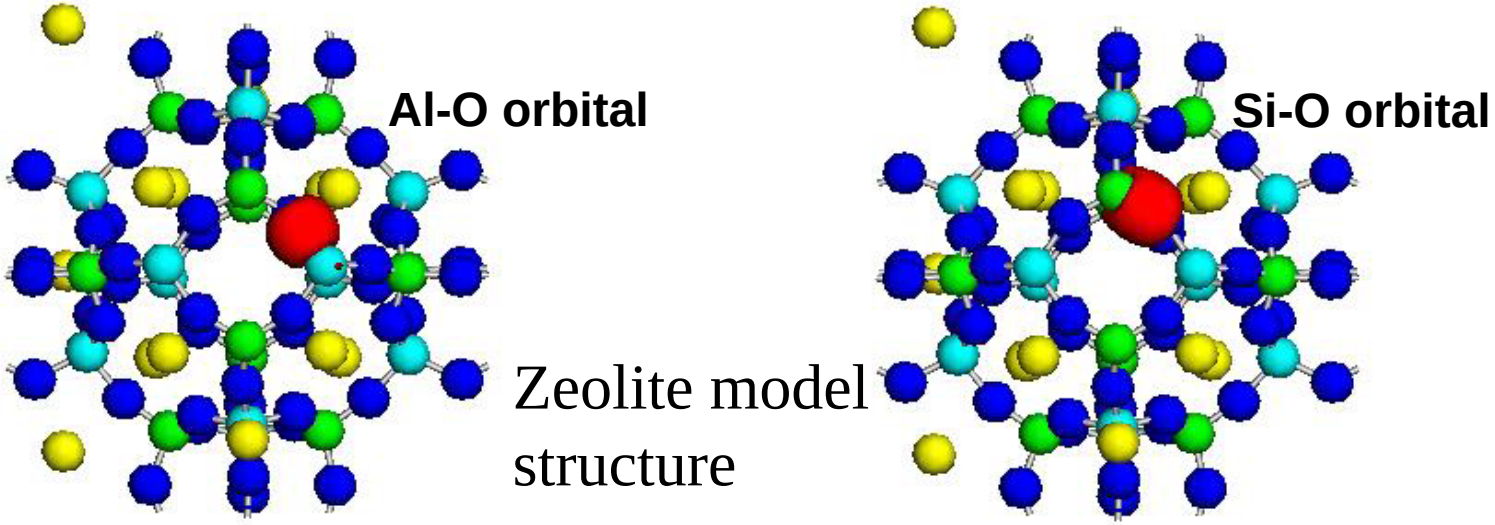
Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

- Issues:
  - Adapting the QDFT method to keep the Green's function matrix manageably small.
  - Energy conservation.
  - QM region needs to be just a few atoms (say, 5) to be able to sample the long times on which collective phenomena occur
    - *Highly dependent on having a good transition.*
  - Update of anchored orbitals in transition region
    - *How often is it needed?*
    - *How accurate does it need to be?*

Modeling Local Chemistry

- First Year's Progress: Efficient GFES method implemented.
- Multiscale method enables study of electron distribution in the structure.

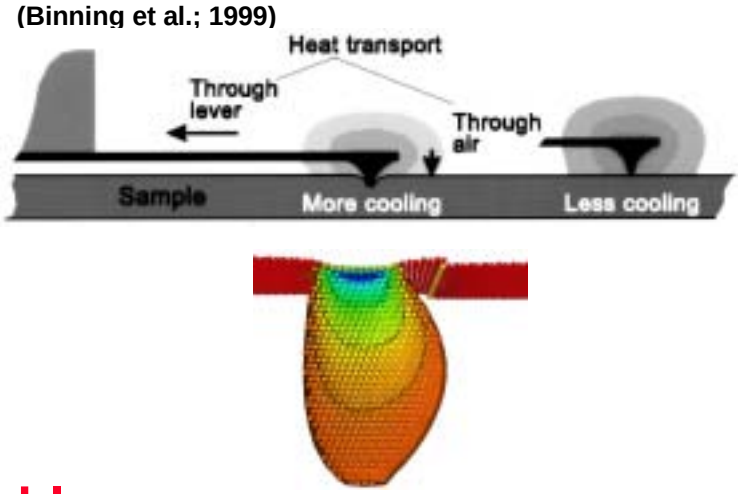


[O: dk blue, Al: lt blue, Si: green, H: red, Na: yellow]

Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

- Advantages:
  - Natural, nearly seamless coupling of QM to MD.
    - *No need to artificially terminate bonds.*
    - *Good balance of comput'l effort between QM & MD.*
  - Thermal energy transfers between regions.
  - Collective Phenom. of MD region influence chemistry in QM region thru transmitted strains and E-Field
  - Good parallel scaling.
  - Amenable to adaptively spawning QM regions.
  - Prototype for class of confined reaction problems
    - *Catalysis*
    - *in vivo reactions (enzyme moderated)*
    - *Reactivity in nanotechnological settings*

A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman



Problem:

Sandia designs and manufactures devices that exhibit multiple modes of material failure, e.g. brittle fracture and plasticity, at various length scales. Models are needed to provide accurate predictions of material reliability.

Aim:

Develop a simulation methodology that contains *atomistics* to model the defect-related mechanisms operating at the nano-scale and *continuum mechanics* to simulate micro- and macro-scale geometries.

Result:

Modeling capability that efficiently and consistently conveys fine-scale detail up to a macroscopic continuum simulation of material response.

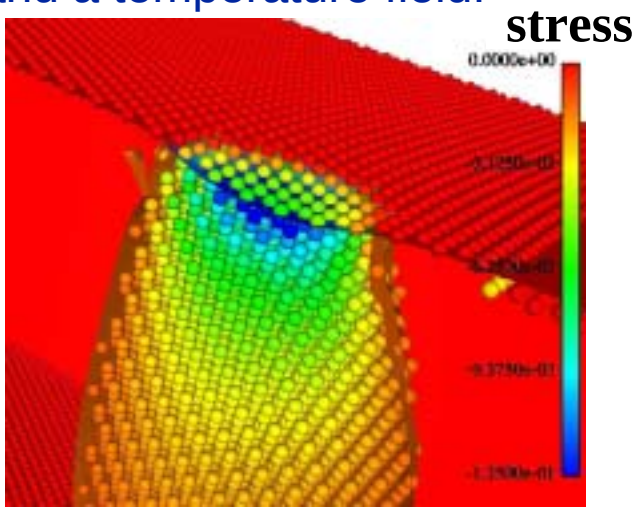
Test Case:

AFM data storage by thermo-mechanical indentation

A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman

Technical Approach:

- Develop compatible definitions for stress, deformation and temperature for both domains.
- Formulate proper interface conditions between the domains.
- Perform an analysis on wavelength-dependent energy content for mechanical deformation of atomistic systems.
- Partition the energy transferred between a dynamic atomistic system and a finite element mesh into elastic waves and a temperature field.



Applications:

- Simulations of experiments used to obtain material properties - e.g. nanoindentation.
- Fundamental understanding of the thermo-mechanical behavior of material defects.
- Mechanical analysis of nano-scale deformation during friction, stiction and wear.

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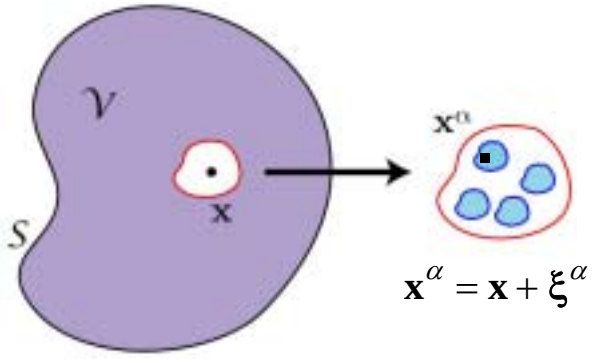
A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman

First Year's Progress:

- Evaluated atomistic definitions of stress for consistency with continuum
- Extended micropolar continuum theory to provide transition between atomistics and continuum:
  - A structured continuum with additional internal degress of freedom.



- Developed a hybrid gridding method to manage load balancing for coupled atomistic-continuum simulations on MP computers.

The Further Challenge: Activated Processes

- Identifying Transition States is the key for capturing Diffusion, Reactivity, and Chemistry in simulations.
- Transition State finding is computionally intensive.
- Transition States determine Chemical Specificity but are dependent on system dynamics (Collective Phenomena)
  - How to couple these in a simulation?
- Transitions are infrequent and sparse
  - Their time and location are not known.
  - Quantum accuracy will be required, usually
- The Next Goal: Adaptively apply QM & find Transition States when and where they are needed within a large, classical MD system.

A Current Challenge for Quantum DFT – Improving Treatment of Many-Body Effects

- QDFT is the workhorse method providing the underpinnings of multiscale materials simulation
- QDFT is exact, . . . in theory.
- Sandia National Laboratories Workshop To spur progress in developing better EXC functionals:

Quantum Mechanical Techniques: Exchange - Correlation Functionals in Density Functional Theory

  - 14-16 August 2002 at the Wyndham Hotel, Albuq.
  - Sponsored by the Computer Science Research Institute and the Physical & Chemical Sciences Center
  - Ann Mattsson, Organizer

THANKS!
to many colleagues for contributions

- Physical & Chemical Sciences, 1100
  - Normand Modine
  - Ann Mattsson
  - Alan Wright, Kevin Leung
  - J. Charles Barbour
  - Neal Shinn
- Materials & Process Sciences, 1800
  - Stephen Foiles
  - Michael Chandross
  - H. Eliot Fang
  - Jeffrey Hoyt
- Engineering Sciences, 9100
  - Bob Chambers
  - James Cox
  - E. David Reedy
  - Arne Gullerud
  - Terry Hinnerichs
- Materials & Engineering Sci.s, 8700
  - Jon Zimmerman
  - Mark Horstemeyer
- Geoscience & Environment, 6100
  - Louise Criscenti
  - Henry Westrich
- Pulsed Power Sciences, 1600
  - Michael Desjarlais
- Computation, Computers, Information & Mathematics, 9200
  - Peter Schultz
  - Steven Plimpton
  - Mark Sears

Coupled Simulation Methods: Transitions

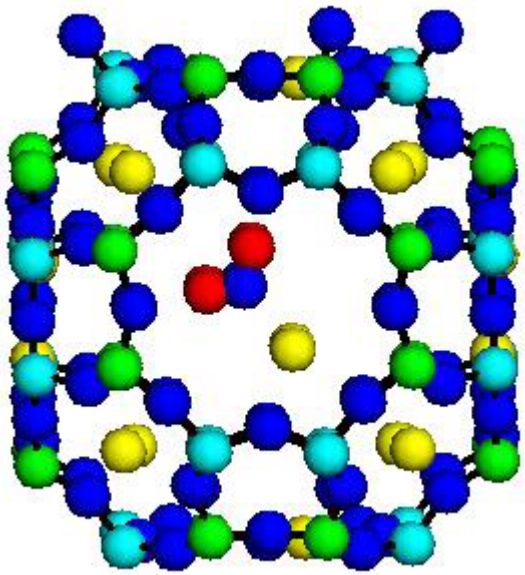
- Scientific insight is required to devise the needed Transitions between scales and methods:
  - Discrete to thermomechanical Continuum
  - Quantum to Classical
  - Deterministic to Statistical/Stochastic
    - *Continuum is implicitly a statistical average*
    - *Stochastic events often used in Mesoscale simulation*
    - *Getting there and back may differ*
      - QM to Molecular Continuum:
        discrete → continuum
      - Molecular Continuum to QM:
        statistical → deterministic

Why is corrosion a concern?

- atmospheric corrosion is the leading degradation mode in the stockpile
  - observed in many components and all weapon systems
  - single largest category of materials-related Significant Finding Investigations (SFI's)
  - typically occurs due to unknowns and/or unexpected changes in environment
- the potential consequence of corrosion in electronics on weapons function is high.

Modeling Local Chemistry I

- QDFT calculation of 14 relaxed, locally stable structures identified 4 likely at room temperature
  - Water binds within 8-oxygen ring rather than inside a pore.
  - Hydrogen bonding or polar character of H_2O implicated.



[O: dk blue, Al: lt blue,
Si: green, H: red, Na: yellow]